# The Importance of Computational Science

Science and engineering have traditionally advanced our knowledge and understanding using several approaches:

**Experimentation** – experimentation has been very important to all aspects of science and engineering. We set up experiments that allow us to control the conditions such that we can connect a **cause** that we specify with an **effect** we can measure. Often, we undertake a large number of experiments so that we are sure we understand the nature of the effects through a wide range of conditions.

**Theory** – theories evolve as we accumulate a large amount of experimental evidence that allows us to generalize our observations. In this sense, theory is connected with experimentation as experiments have been completed or can be formulated to test our theories. Some theories arise as conjectures by scientists that must be tested with experimentation. Others are widely tested and are unlikely to change. When a high degree of certainty is ascribed to a theory based on widespread testing, we sometimes call that a **law**. An example is Newton's laws of motion.

As scientists and engineers work to understand and build increasingly complex systems, experimentation may not be adequate to test emerging theories. This can be for a number of reasons:

- The phenomenon may be too small too small to see and adequately instrument to be effectively measured. This is the case for work at the atomic or subatomic level and for engineering nano-scale devices.
- The systems being studied are too large and remote to devise an experiment. This is the case in the study of galaxies and other aspects of cosmology.
- The process may happen too fast or be too complex to effectively measure all of the intermediate steps that occur in the cause and effect chain. For many biological processes this is the case as simultaneous biochemical processes occur in plants and animals. This may also be the case for complex engineered systems where there are multiple interactions among components and therefore a huge number of potential outcomes.
- Experimenting on the system would cause harm we wish to avoid. For example, we don't want to experiment on a watershed to see how much pollution it takes to wipe out a particular fish species or cause human disease when the water is consumed.

**Modeling and Simulation**
Several of these limitations apply for many engineering processes and programs. In addition, traditional approaches to designing systems and products, building and testing prototypes, and arriving at a final product are no longer sufficient for firms to stay competitive in the global market. With a design in mind, the building of a prototype is a very expensive process and takes a long time. Those things result in an increase in the cost of product development, a delay in getting products to market, and a limitation on innovation as few companies can afford to build more than a few prototypes and test a few designs. Thus there are substantial benefits to industry for adopting computational modeling as a part of their design, product development, and management processes:

- Virtual prototypes, models of products or processes done with computer simulation, can greatly reduce or even eliminate the need to build physical prototypes, saving a great deal of money in the development process.
- Many more alternatives can be examined using computer modeling, spurring more innovative, more efficient, and more salable final products.

- Computer modeling saves a great deal of time in examining alternatives, making it possible to make changes in current products or to bring new products to market more rapidly. This provides an important competitive advantage for the businesses that use this approach.
- Simulation results can be shared within an organization, allowing timely feedback among engineers, designers, marketing, and other people in a firm and assuring that the final product will meet multiple goals.

**Readings and Exercise**

**Part 1** Below are pointers to reports that document the value of computational science to science and engineering discovery. Each student should read the executive summaries of these reports. Focus mostly on the general purpose of the studies and how they related to the principles discussed above rather than the final recommendations of the authors.

**PITAC Report to the President**
http://www.nitrd.gov/pitac/reports/20050609_computational/computational.pdf#search=%22committee%20on%20competitiveness%22

**National Science Foundation (NSF)**
**Science Based Engineering Science (SBER Report)**
http://www.nsf.gov/pubs/reports/sbes_final_report.pdf#search=%22simulation%20based%20engineering%20science%22

**World Technology Evaluation Center, Inc.**
**Research Directions Workshop**
http://www.nsf.gov/mps/ResearchDirectionsWorkshop2010/RWD-color-FINAL-usletter_2010-07-16.pdf

**Part 2** Read about a real example of how a model is used to aid discovery, design, product development, or business competitiveness. Write a 1-2 page summary of the example to share with your classmates using the framework below. If your example does not cover a particular subtopic, indicate that in your write-up as "Not Applicable".

Choose one item at random from the list below by going to http://www.mathgoodies.com/calculators/random_no_custom.html and choosing a number between 1 and 18. Read about that item from the list below and fill in the report. You will upload your brief report to the discussion group for this topic. You will also be required to read the reports from your classmates.

1. Monitoring the US Economy – Starting on page 62 of the PITAC report.
2. Discovering Brown Dwarves via Data Mining – Starting on page 69 of the PITAC report
3. Modeling Real-Time Complex Systems in the Human Environment – Starting on page 72 of the PITAC report
4. Dynamic Modeling of the Spread of Infectious Disease – Starting on page 73 of the PITAC report
5. Predicting severe storms - http://www.psc.edu/science/2004/droegemeier/retwistered_twister.php
6. Discovering oil reserves - http://access.ncsa.uiuc.edu/Stories/oil/
7. Modeling Ozone levels in the atmosphere - http://www.epa.gov/scram001/modelingapps_photo.htm Read the slide set from the first link. This one contains a lot of lingo so you may need to refer to this site or ask for help to translate: http://www.epa.gov/air/caa/peg/
8. Toyota uses MATLAB for design http://www.mathworks.com/industries/auto/userstories.html?file=2340

9. Breakthroughs in Brain Research http://www.compete.org/publications/detail/503/breakthroughs-in-brain-research-with-high-performance-computing/
10. Auto crash safety http://www.compete.org/publications/detail/390/grand-challenge-case-study-auto-crash-safety/
11. Vehicle design http://www.compete.org/publications/detail/388/grand-challenge-case-study-vehicle-design/
12. Delphi horizontal modeling http://www.autonews.com/assets/html/10_pace/winners/2004_Delphi_Corporation.html
13. P&G Bottle Design http://phx.corporate-ir.net/phoenix.zhtml?c=104574&p=irol-newsArticle&ID=651774&highlight= and http://www.scienceinthebox.com/en_UK/sustainablehome/4_2_2.html
14. Competition in refrigeration http://www.ansys.com/magazine/issues/2-1-2008-rotating-machinery/03-consumer-products.pdf
15. Glass industry http://www.ansys.com/magazine/issues/2-1-2008-rotating-machinery/05-mat-submerged.pdf
16. U.S. Air Force training http://www.afams.af.mil/shared/widgets/popup.asp?url=http://www.afams.af.mil/shared/xml/rssVideo.asp?mrsstype=2&id=207&cid=250&pos=0
17. Auto racing http://www.fluent.com/solutions/sports/tn272.pdf
18. Pet food manufacturing http://www.fluent.com/solutions/food/CS105-wenger.pdf